# SPECTROSCOPIA MOLECULAR

Un bulletin mensual de novas e informationes de interesse e valor al spectroscopistas molecular

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IO CREDE QUE omne le fines, le objectivos, e le activitates de un universitate pote esser focalisate si nos lo considera como primarimente un centro de pensata creative. Il es un truismo que omne le cambiamentos de civilisation, omne le cambiamentos in le maniera in le qual nos vive e pensa, es le resultatos del pensar creative de homines e feminas individual.

-- L. A. DuBRIDGE, Presidente, Instituto Technologic de California. (Ex un discurso excellente super "Le Fines del Recerca Universitari", publicate in Electrical Engineering, le Journal of Engineering Education, e le Addison-Wesley Newsletter.)

## NOVE DISVELOPPAMENTOS

**PARAFFINES NORMAL. Assignationes de frequentias in le region 650-1450 K ha essite satisfacentemente facite. (H. TSCHAMIER, J. Chem. Phys. 22, 1845-1854 (1954); Prime Instituto Chimic, Universitate Vienna, Austria.)

* * *

**ALKYLSILANOS. Ha essite preparate e purificate 12 alkylsilanos, includente omne le homologias de methylo e ethylo. Spectros infrarubie de illus ha essite obtenite. (S. KAYE e S. TANNENBAUM, J. Org. Chem. 18, 1750-1754 (1953); Lewis Flight Propulsion Laboratory, National Advisory Committee for Aeronautics, Cleveland 11, Ohio, Statos Unite.)

* * *

**PROBABILITATES DE TRANSITION. Istos es de importantia in studios del composition chimic de objectos astronomic, proque illos face possibile le determination de temperaturas de excitation, e assi le abundantias molecular relative. Resultatos ha essite experimentalmente obtenite usque nunc pro $C_2$, TiO, VO, CaH, MgO, e YO. De plus, le moleculas ZrO, CH, CN, e MgH ha essite observate photoelectricamente. (J. PHILLIPS, Mémoires in-8° de la Société Royale des Sciences de Liége, Quatrième Série, Tome XIII, Fasc. III, 452-459; Universitate California, Berkeley, S. U.)

* * *

**CAMBIAMENTO DE POLARISABILITATE. Valores median del rata de cambiamento del polarisabilitate con le distantia internucleari esseva determinate ex le ration del intensitates Raman e Rayleigh in le gas. Illos es:

| | | |
|---|---|---|
| $H_2$ | 1,2 . $10^{-16}$ | $cm^2$ |
| $D_2$ | 1,1 | " |
| HCl | 1,1 | " |
| HBr | 1,2 | " |
| $N_2$ | 1,6 | " |
| $O_2$ | 1,4 | " |
| $CO_2$ ($\sigma_1$) | 4,2 | " |
| $CH_4$ ($\sigma_1$) | 4,1 | " |

Le valores pro le moleculas partialmente ionic HCl e HBr es proxime a los de $H_2$ e $D_2$. (E. J. STANSBURY, M. F. CRAWFORD, e H. L. WELSH, Can. J. Phys. 31, 954-961 (1953); Laboratorio McLennan, Universitate Toronto, Toronto, Canada.)

* * *

**FACTORES DE DISPOLARISATION. Calculation del factores de dispolarisation del lineas Raman de moleculas polyatomic ha essite considerate. Expressiones general pro le tensor de polarisabilitate derivate es deducite pro moleculas non-cyclic que ha ligamines con symmetria cylindric. Assumite es le additivitate del polarisabilitates de ligamine como proponite per Wolkenstein. Le technica de matrices F e G introducite per E. B. Wilson, Jr., es usate. Como exemplo, le expressiones pro le tracia (summa del elementos diagonal de matrice) e le anisotropia pro le typo molecular $CX_3Y$ es explicitemente obtenite. (S. M. FERIGLE e A. WEBER, Can. J. Phys. 32, 799-807 (1954); Instituto Technologic de Illinois, Chicago 16.)

* * *

**VELOCITATE DE LUMINE. Le constante rotational $B_{000}$ de HCN es 1,47823$_5$ K. Isto esseva obtenite per le methodo de ordines exacte (Rank, Shull, Bennett, e Wiggins, J. Opt. Soc. Am. 43, 952 (1953)) pro le banda de absorption vibrational rotational infrarubie 002. Combinate con le mesurationes microundic de Nethercot e Klein del mesme constante in unitates de frequentia pur, isto dava 299789,8 ± 3,0 km/sec como velocitate de lumine. (D. H. RANK, J. N. SHEARER, e T. A. WIGGINS, Phys. Rev. 94, 575-578 (1954): Universitate Statal de Pennsylvania, State College, Pa., Statos Unite.)

* * *

**ANULO CYCLOPROPYLIC. Le region 9,5-10,0 μ es le melior pro le determination del anulo cyclopropylic. Cata un de 34 compositos que contineva iste gruppo absorbeva fortemente in iste region. Quando resolution adequate pote esser obtenite, le bandas anulic C-H a 3,23 e 3,32 μ confirma le presentia del anulo. (V. A. SLABEY, J. Am. Chem. Soc. 76, 3604 (1954); Lewis Flight Propulsion Laboratory, Cleveland 11, Ohio, S. U.)

# TRACTAMENTOS DEL COORDINATAS NORMAL DE MOLECULAS POLYATOMIC
## B. APPLICATIONES SPECIFIC

Forrest F. Cleveland, Arnold G. Meister, e Fred L. Voelz
Instituto Technologic de Illinois, Chicago 16, Illinois

(continuate ab Spec. Mol. 4, 17 (1955))

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## 2B. Le Matrices F

PRO OBTENER le equationes ex le quales le frequentias vibrational pote esser determinate, il es necessari calcular le elementos de un matrice F associate con le energia potential, e un matrice G associate con le energia cinetic. Pro motion harmonic de parve amplitude, le energia potential V pote esser scribite como[6]

$$2V = \sum f_{ik}\, r_i\, r_k; \qquad (2B1)$$

$f_{ik} = f_{ki}$ e i e k se extende a omne le coordinatas interne. Pro $H_2O$, isto deveni

$$2V = f_d(\Delta d_1^2 + \Delta d_2^2) + f_\alpha \Delta\alpha^2 + 2f_{d\alpha}(\Delta d_1 + \Delta d_2)\Delta\alpha + 2f_{dd}\Delta d_1 \Delta d_2. \qquad (2B2)$$

In terminos del coordinatas de symmetria, V pote esser scribite como

$$2V = \sum F_{jl}\, S_j\, S_l. \qquad (2B3)$$

Hic etiam, $F_{jl} = F_{lj}$ e j e l se extende a omne le coordinatas de symmetria S.

In le notation de matrice,[7] Eqs. 2B1 e 2B3 deveni

$$2V = r'fr \qquad (2B4)$$

e

$$2V = S'FS; \qquad (2B5)$$

r' e S' es le transpositiones del matrices r e S respectivemente. Ex iste equationes, nos ha

$$r'fr = S'FS. \qquad (2B6)$$

Exsection 2A

$$S = Ur \qquad (2B7)$$

o

$$r = U^{-1} S, \qquad (2B8)$$

ubi $U^{-1}$ es le inverso de U. Sed proque le $S_j$'s es orthogonal e normalisate, $U^{-1} = U'$. Assi Eq. 2B8 deveni

$$r = U'S \qquad (2B9)$$

e

$$r' = (U'S)' = S'U, \qquad (2B10)$$

proque le transposition de un producto es equal al producto del transpositiones prendite in le ordine reverse. Assi Eq. 2B6 pote esser scribite como

$$S'(UfU')S = S'FS \qquad (2B11)$$

si que

$$F = UfU'. \qquad (2B12)$$

Isto es le relation que es necessari pro obtener le matrice F.

Pro $H_2O$ le matrice f es (Eq. 2B2)

| | $\Delta d_1$ | $\Delta d_2$ | $\Delta\alpha$ |
|---|---|---|---|
| $\Delta d_1$ | $f_d$ | $f_{dd}$ | $f_{d\alpha}$ |
| $\Delta d_2$ | $f_{dd}$ | $f_d$ | $f_{d\alpha}$ |
| $\Delta\alpha$ | $f_{d\alpha}$ | $f_{d\alpha}$ | $f_\alpha$ |

e le matrice U pro le vibrationes de $a_1$ es (Eqs. 2A1 e 2A2)

| $a_1$ | $\Delta d_1$ | $\Delta d_2$ | $\Delta\alpha$ |
|---|---|---|---|
| $S_1$ | $2^{-\frac{1}{2}}$ | $2^{-\frac{1}{2}}$ | 0 |
| $S_2$ | 0 | 0 | 1 |

Per consequente, U' es

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[6] Vide E. T. Whittaker, Analytical Dynamics (Cambridge, ed. 2, 1927), p. 178.

[7] Pro un introduction a matrices, vide H. Margenau e G. M. Murphy, The Mathematics of Physics and Chemistry (Van Nostrand, 1943), p. 288.

$$\begin{pmatrix} 2^{-\frac{1}{2}} & 0 \\ 2^{-\frac{1}{2}} & 0 \\ 0 & 1 \end{pmatrix}.$$

Assi fU', obtenite per le multiplication del matrices f e U', es

$$\begin{pmatrix} 2^{-\frac{1}{2}}(f_d + f_{dd}) & f_{d\alpha} \\ 2^{-\frac{1}{2}}(f_d + f_{dd}) & f_{d\alpha} \\ 2\, f_{d\alpha} & f_\alpha \end{pmatrix}.$$

Ex Eq. 2B12, le matrice F es

$$\begin{pmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{pmatrix} a_1 = \begin{pmatrix} f_d + f_{dd} & 2\, f_{d\alpha} \\ 2\, f_{d\alpha} & f_\alpha \end{pmatrix} a_1.$$

Pro le vibration de typo $b_1$,

$$U = (2^{-\frac{1}{2}} \quad -2^{-\frac{1}{2}} \quad 0) \qquad U' = \begin{pmatrix} 2^{-\frac{1}{2}} \\ -2^{-\frac{1}{2}} \\ 0 \end{pmatrix}$$

Assi

$$fU' = \begin{pmatrix} 2^{-\frac{1}{2}}(f_d - f_{dd}) \\ 2^{-\frac{1}{2}}(f_{dd} - f_d) \\ 0 \end{pmatrix}$$

e

$$F = (F_{33})^{b_1} = (f_d - f_{dd})^{b_1}.$$

Iste caso es multo simple proque il ha solmente un elemento de matrice.

(Va continuar in un numero futur)

* * *

## REVISTAS

Theoria de Structura Molecular e Spectros. A. D. WALSH, Ann. Rev. Phys. Chem. 5, 163-184 (1954). Departimento de Chimia, Universitate Leeds, Leeds, Anglaterra.

* * *

Theoria Quantic de Valentia. H. C. LONGUET-HIGGINS, Ann. Reports Chem. Soc. 48, 7-16 (1951). Universitate Cam-

(continuate al pagina 25)

## NOVE LIBROS

The Strengths of Chemical Bonds (Le Fortias de Ligamines Chimic). T. L. COTTRELL. Academic Press, 125 E. 23rd St., New York 10, N. Y.; Butterworths Scientific Publications, London, 1954. 310 + viii paginas. $5.50.

DISCUTITE IN DETALIO es le methodos experimental de determinar le energias de dissociation de moleculas diatomic e polyatomic, tanto como le methodos de obtener le calores de formation de moleculas. Tabulate es le valores numeric del calores de atomisation, distantias internucleari, e constantes de fortia.

* * *

Introduction to Statistical Thermodynamics (Introduction al Thermodynamica Statistic). MALCOLM DOLE. Prentice - Hall, 70 5th Ave., New York 11, 1954. 250 + xii paginas. $6.25

UN NOVE TRACTAMENTO basic que ponta le brecha inter thermodynamica e cinetica de un latere, e chimia e physica del altere. Le fundamentos del thermodynamica es revidite e le principios del mechanica statistic es presentate. Tunc passo a passo es demonstrate como le duo subjectos es relatate in le thermodynamica statistic. Applicationes specific e practic de iste principios es includite.

* * *

Tractamentos del Coordinatas Normal de Moleculas Polyatomic. SALVADOR M. FERIGLE e ALFONS WEBER (traducite e redigite per Forrest F. Cleveland. Publicate per Forrest F. Cleveland). c/o Laboratorio de Spectroscopia, Instituto Technologic de Illinois, Chicago 16, 1955. 25 + v paginas. $1.00 nette.

ISTO ES LE 2nde de un serie de parve monographias super spectros molecular. (Le 1me monographia tractava del regulas de selection pro spectros vibrational de moleculas polyatomic.) Le presente volumine explica le theoria general de tal tractamentos. Le formulas es derivate e applicate al $XY_2$ linear e nonlinear, tanto como $CX_3Y$ tetrahedric. Le conditiones Eckart es discutite e le uso del symmetria del molecula pro simplificar le problema es demonstrate.

## SUMMARIOS DE ARTICULOS FUTUR

Studio de Chelation per le Effecto Raman. P. G. PURANIK Laboratorios Physic, Universitate Osmania, Hyderabad, India. Submittite al J. Chem. Phys. le 1 de februario 1955.

DISPLACIAMENTOS RAMAN obtenite pro salicylaldehydo es: 151(5b), 268(6), 299(2), 413(4), 453(8), 565(7), 669(2), 773(0), 890(1), 1033(8), 1120(3), 1154 (7), 1230(9), 1282(4), 1324(10), 1378 (2), 1462(10), 1581(8), 1623(6), 1648 (6), 1669(9), 3057 ± 23 (1b). Le linea C=O in le aldehydo pur e in mixturas con phenol e alcohol methylic habeva le sequente displaciamentos:

| | |
|---|---|
| Salicylaldehydo pur.... | 1669 |
| Mixtura con phenol | |
| 1 : 0,5 (per vol.).... | 1669 |
| 1 : 1 ..... | 1674 |
| Mixtura con alcohol methylic | |
| 1 : 1 ..... | 1675 |
| 1 : 4 ..... | 1672 |
| 1 : 9 ..... | 1670 |

Le resultatos in iste caso es le reverso de illos pro ketonos, aldehydos, e esteres miscite con solventes acceptoric. Isto suggere que le fortia de chelation es opponite per le fortia del ligar hydrogenic intermolecular con le phenol o alcohol.

Assi, salicylaldehydo es un exemplo del transition ex ligar hydrogenic intramolecular al ligar hydrogenic intermolecular, como demonstrate per le effecto Raman.

## TRADUCTIONES

TRADUCTIONES in anglese de articulos russe, francese, german, e espaniol es disponibile a $10 per 1000 parolas. Etiam disponibile es traductiones in anglese de plure jornales russe. Abonamentos a istos es $80 a $95 per anno. Le jornales es primarimente chimic. Pro plus informationes, scribe a E. M. Coleman, Consultants Bureau, 152 W. 42nd Street New York 18, N. Y., Statos Unite.

## SUMMARIOS DE ARTICULOS RECENTE

Constantes Spectroscopic de Moleculas I. Frequentias pro le Stato le Plus Basse de Diatomos $X_2$. K. MAJUMDAR e Y. P. VARSHNI, Indian J. Phys. 28, 103 (1954). Departimento de Physica, Universitate Allahabad, Allahabad, India.

EVALUTATION THEORIC del constantes spectroscopic de moleculas per le mechanica quantic ha essite retardate a causa del difficultates in le calculationes. In iste serie, le presente relationes inter le constantes spectroscopic va esser discutite, e nove relationes empiric o semitheoric essera proponite.

Un melior forma del relation Matuyania-Clark es proponite. Isto es

$$\log \omega_e = g - h \log n^2 V;$$

$\omega_e$ es le frequentia, g e h es constantes pro cata gruppo, n es le numero quantic principal, e V es le potential de ionisation. Predicite es valores pro $Fr_2$, $Ge_2$, $Sn_2$, $Po_2$, e $At_2$.

Es proponite que le unitate "$10^5$ dynas/cm" sia appelate "deslandre (des.)" in honor de Deslandre.

* * *

II. Frequentias Vibrational de Diatomos XY. K. MAJUMDAR e Y. P. VARSHNI, ibid., 28, 209 (1954).

HA ESSITE STUDIATE le relation del frequentia vibrational de XY con illos de $X_2$ e $Y_2$, in le qual X e Y pertine al mesme gruppo del tabula periodic. Si $\omega_e^{0,65}$ pro XY es representate per $\phi(XY)$ tunc il es trovate que

$$\phi(XY) = \left[\phi(XX) + \phi(YY)\right]/2.$$

Valores calculate e observate es in bon concordantia. Multe frequentias ha essite predicite.

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REVISTAS (continuate ab pagina 24)

bridge, Cambridge, Anglaterra.

* * *

Structura Molecular. C. A. McDOWELL, Ann. Reports Chem. Soc. 48, 16-38 (1951).

## CALENDARIO 7

April 4-6. Symposio del Societate Faraday super spectroscopia microundic e frequentias radionic. Cambridge, Anglaterra. (Plus detalios in le numeros currente del Trans. Faraday Soc.)

Maio 6. Association American de Spectrographos, 6te conferentia annual, in Chicago, Applicationes industrial de spectroscopia. Spectros emissionic e absorptionic, e del fluorescentia de spectroscopia. Spectros emissionic e absorptionic, e del fluorescentia de radios x. (F. Stedman, Corporation Bendix Aviation, 401 Bendix Drive, South Bend 20, Indiana, Statos Unite.)

Maio 26-27. Societate pro Spectroscopia Applicate, 10me symposio annual e exhibition, New York.

Junio 13-17. 10me symposio annual super spectroscopia e structura molecular. (H. H. Nielsen, Departimento de Physica, Universitate Ohio State, Columbus 10, Ohio, Statos Unite.)

Julio 7-11. Convention de Spectroscopistas Molecular Europee, Oxford, Anglaterra. Spectroscopia ultraviolette absorptionic, Raman e infrarubie includente nove disveloppamentos in tecnicas, spectros vibrational de moleculas complexe, mesurationes con alte resolution, spectros de flammas, campos de fortia, spectros de crystallos, e le infrarubie remote. (H. W. Thompson, St. John's College, Oxford, Anglaterra.)

Julio 18-29. Programma intensive de spectroscopia infrarubie. (R. C. Lord, Laboratorio de Spectroscopia, Instituto Technologic de Massachusetts, Cambridge Massachusetts, Statos Unite.)

Septembre 14-16. 2nde symposio Ottawa super spectroscopia applicate. (J. K. Hurwitz, Branca de Minas, 568 Booth St. Ottawa, Ontario, Canada.)

Junio 1956. Convention del Commission Juncte pro Spectroscopia. Columbus, Ohio o Washington, D. C., S.U. (W. F. Meggers, Bureau National de Standards, Washington 25, D. C., Statos Unite.)

### STATISTICA VITAL

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SPECTROSCOPIA MOLECULAR es redigite e publicate mensualmente in Interlingua per Prof. Forrest F. Cleveland, Laboratorio de Spectroscopia, Instituto Technologic de Illinois, Chicago 16, Illinois, Statos Unite. Manuscriptos pro publication debe esser submittite illac.

Le texto original es legite per Dr. Alexander Gode, Chef del Division de Interlingua de Science Service (80 East 11th St., New York 3, N.Y.) Libros importante super Interlingua, disponibile ab ille adresse, es Interlingua-English Dictionary, Interlingua Grammar, e Interlingua A Prime Vista.

Labor editorial es gratis. Le costo de preparation e distribution es recipite ab spectroscopistas, bibliothecas, e companias. Assistentes de publication es Stta. Ruth Grining e Sr. Jerome M. Dowling. Le imprimer es facite per le Servicios de Bureau al I. T. de Ill. sub le direction de Stta. Virginia Brown.

### DISPONIBILE

1. Spectroscopia Molecular, 12 numeros per anno, $2.00 nette, franc de posta.
2. Volumines passate de Spec. Mol. pro le annos 1952, 1953, e 1954; $3.00 nette per cata un, franc de posta.
3. Numeros individual, $0.25 per cata un.
4. Monographias super Spectros Molecular. I. Regulas de Selection pro Spectros Vibrational de Moleculas Polyatomic, Forrest F. Cleveland, 1953. 25 paginas, $0.75 nette.
5. II. Tractamentos del Coordinatas Normal de Moleculas Polyatomic, Salvador M. Ferigle e Alfons Weber, 1955. 30 paginas, $1.00 nette.
6. Companias pote attachar un pagina de informationes in re lor productos al sequente numero, si illos es de interesse a spectroscopistas molecular.
7. Spectroscopistas pote requestar le addition de lor nomines al lista de membros del Societate del Spectroscopistas Molecular. Il ha nulle quotas, sed parve contributiones pote esser facite pro expensas necessari.

(Face cheques pagabile a Spectroscopia Molecular e posta al supra-date adresse.)

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# INSTRUMENT DIGEST

A condensation of some articles in the Winter issue of THE PERKIN-ELMER *INSTRUMENT NEWS*, a publication of The Perkin-Elmer Corporation, manufacturers of scientific instruments--Infrared Spectrometers, Tiselius Electrophoresis Apparatus, Monochromators, Flame Photometers, Continuous Infrared Analyzers, Vernistats, Amplifiers, Astronomical Equipment, Thermocouples, Lenses, Crystal Optics, Special Designs for the Government.
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Norwalk, Conn. April, 1955 Vol. 6, No. 2

## TRI-NONs MONITOR PROCESS STREAMS AT CYANAMID'S NEW FORTIER PLANT

Principal product of the new $50,000,000 American Cyanamid plant at Fortier, La. is acrylonitrile, with ammonia and acetylene as important by-products and intermediates. Nearly a dozen Perkin-Elmer TRI-NON* Analyzers are now on the line to provide continuous analytical information to the operators of the various units.

In the ammonia unit, for example, four low range (0-50 ppm) TRI-NONs monitor CO and $CO_2$ in the feed streams to the reactor to warn against the possibility of catalyst poisoning. Other instruments keep tabs on various phases of acetylene production and purification.

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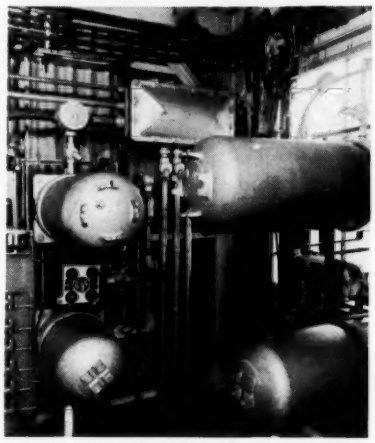

TRI-NONs *monitor ammonia and acetylene process streams at Fortier.*

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● **Functional** – The redesigned front panel presents a clean, modern, uncluttered look. The sloping front allows all meters and indicators to be read and adjusted quickly and easily from a sitting position. Knurled wheels on the front panel control operation of the internal standard measuring adjustments for comparing sample with standard. These knobs are controlled by thumb movement with the hands resting comfortably on the top, reducing operator fatigue and resulting in more accurate routine analyses. All readings are done at a glance from numerical indicators.

Atomizer and burner of the Model 146 are readily disassembled for simple servicing. The top, back and sides of the instrument come off as a single unit, quickly exposing all parts for inspection or replacement.

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